Path Integral for a Particle in a Box

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M275
Spring, 1994

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<u>Summary</u>: Starting with the Schrödinger wave equation we calculate the propagator for the 1-dim free particle in a box. By using theta function identities, this is represented as a sum over paths. The sum involves the free particle propagator on $\mathbb{R}^1$ and a nonabelian, discrete affine group. An interpretation of the formula is suggested.

1. The Classical QM propagator

Let $a > 0$, $I = [-a, a] \subseteq \mathbb{R}$. Let B denote the classical mechanical system, defined on I with Lagrangian

$$L(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - V(x), \quad \text{where} \quad V(x) = \begin{cases} 0 & x \in (-a, a) \\ \infty & x \in \{-a, a\} \end{cases}$$

We think of B as a limit of classical systems, $B = \lim_{N \to \infty} B_N$, where B_N is defined on $\mathbb{R}$ with Lagrangian

$$L_N(x, \dot{x}) = \frac{1}{2}\dot{x}^2 - V_N(x), \quad V_N(x) = \begin{cases} 0 & x \in (-a, a) \\ N & \text{otherwise} \end{cases}$$

(or we may take V_N to be continuous, eg:

Let $Q(X)$ denote "quantization" of the system X.
Then we define $Q(B) = \lim_{N \to \infty} Q(B_N)$, where $Q(B_N) =$ standard Schrödinger quantization of B_N on $\mathbb{R}$.

Elementary arguments show that the stationary solutions for $Q(B)$ must satisfy:

$$-\frac{\hbar^2}{2}\frac{d^2 u}{dx^2} = E u \quad \text{for } |x| < a, \text{ and } u(-a) = u(a) = 0 \tag{1.1}$$

This has normalized solutions:

$$u_n(x) = \frac{1}{2\sqrt{a}}\left(e^{\frac{i n \pi x}{2a}} + (-1)^{n+1} e^{-\frac{i n \pi x}{2a}}\right) \quad \text{with} \tag{1.2}$$

$$E_n = \frac{\pi^2 \hbar^2 n^2}{8a^2} \qquad n = 1, 2, 3, \ldots$$

Let $K_t(x,y)$ be the propagator for (1.1). Then, by definition, if $u(x,t)$ = solution at time $t>0$ of the time dependent equation:

$$(1.3) \qquad i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi$$

with initial condition $u(x,0)$, we have

$$(1.4) \qquad u(x,t) = \int_I K_t(x,y)\, u(y,0)\, dy \, .$$

Formally, we may write

$$(1.5) \qquad K_t(x,y) = \sum_{n=1}^{\infty} u_n^*(y)\, u_n(x)\, e^{-iE_n t/\hbar}$$

. This follows by seperation of variables in the full equation (1.3) and using Sturm-Liouville theory to deduce completeness of the u_n's for L^2-expansions for solutions to (1.1). Presumably because of 2 cond's. Note that if $H = \overline{\text{span}\langle u_n \rangle}$ in $L^2(I)$, then codim $H = 2$. This creates an ambiguity in the expression for $K_t(x,y)$ - we can add terms belonging to $H^\perp$ without changing the formula (1.4). (since $u(y,0) \in H$).

Consider the term $e^{-iE_n t/\hbar} = \exp\left[\frac{\pi^2\hbar}{8a^2} \frac{t}{i} n^2\right]$

If we treat t as a complex variable, then it is easy to see that the series for $K_t(x,y)$ is abs. and uniformly convergent for $x,y \in I$, for $\text{Im}(t) < 0$. Thus, to rigorously interpret (1.5), we should view it as a limit as $t \mapsto$ real-axis from the lower half plane (alternately, one can consider complex mass terms as in Nelson [3]). Having mentioned this, we shall put this delicate issue aside and assume that all subsequent manipulations (e.g. rearrangements of the sum) can, in the end, be justified.

2. Theta function computations

We expand (1.5) using (1.2):

$$K_t(x,y) = \frac{1}{4a} \sum_{n=1}^{\infty} \left(e^{-\frac{in\pi y}{2a}} + (-1)^{n+1} e^{\frac{in\pi y}{2a}}\right)\left(e^{\frac{in\pi x}{2a}} + (-1)^{n+1} e^{-\frac{in\pi x}{2a}}\right)$$
$$\times \quad e^{-\frac{\pi^2 \hbar i t}{8a^2} n^2}$$

$$= \frac{1}{4a} \sum_{n=1}^{\infty} \left[\exp\left(\frac{\pi i n}{2a}(x-y)\right) + \exp\left(-\frac{\pi i n}{2a}(x-y)\right)\right] e^{-\frac{i\pi^2 \hbar t}{8a^2} n^2}$$
$$- \frac{1}{4a} \sum_{n=1}^{\infty} (-1)^n \left[\exp\left(\frac{\pi i n}{2a}(x+y)\right) + \exp\left(-\frac{\pi i n}{2a}(x+y)\right)\right] e^{-\frac{i\pi^2 \hbar t}{8a^2} n^2}$$

(2.1)
$$= \frac{1}{4a} \sum_{n=-\infty}^{\infty} e^{\frac{\pi i (x-y)}{2a} n} \; e^{-\frac{i\pi^2 \hbar t}{8a^2} n^2}$$
$$- \frac{1}{4a} \sum_{n=-\infty}^{\infty} (-1)^n \, e^{\frac{\pi i (x+y)}{2a} n} \; e^{-\frac{i\pi^2 \hbar t}{8a^2} n^2}$$

Recall the following definitions:

(2.2)
$$\theta_3(z,\tau) = \sum_{n=-\infty}^{\infty} e^{\pi i \tau n^2} e^{2niz}, \quad z \in \mathbb{C} \quad \mathrm{Im}(\tau) > 0$$
$$\theta_4(z,\tau) = \sum_{n=-\infty}^{\infty} (-1)^n e^{\pi i \tau n^2} e^{2niz} \qquad ''$$

We have the basic identities:

(2.3)
$$\theta_3(z+\pi,\tau) = \theta_3(z,\tau), \quad \theta_3(z+\pi\tau,\tau) = e^{-\pi i \tau} e^{-2iz}\theta_3(z,\tau)$$
$$\theta_4(z,\tau) = \theta_3\left(z+\frac{\pi}{2},\tau\right), \quad \text{and a}$$

(2.4) Fundamental Identity: $\theta_3(z,\tau) = (-i\tau)^{-1/2} e^{z^2/\pi i \tau}\, \theta_3\left(\frac{z}{\tau}, -\frac{1}{\tau}\right)$

(Bellman [1])

Thus we write (2.1) as

(2.5)
$$K_t(x,y) = \frac{1}{4a}\,\theta_3\left(\frac{\pi(x-y)}{4a}, -\frac{\hbar\pi t}{8a^2}\right) - \frac{1}{4a}\,\theta_4\left(\frac{\pi(x+y)}{4a}, -\frac{\hbar\pi t}{8a^2}\right)$$

(4) Particle in a Box (cont.) Aaron Hirshman

Consider the expression $\frac{1}{4a}\Theta_3\left(\frac{\pi w}{4a}, -\frac{\hbar\pi t}{8a^2}\right)$

$= \frac{1}{4a}\theta_3(z,\tau)$, $z = \frac{\pi w}{4a}$ $\tau = -\frac{\hbar\pi t}{8a^2}$. Applying (2.4):

$(-i\tau)^{-1/2} = \left(\frac{8a^2}{\pi i\hbar t}\right)^{1/2}$, $\frac{z^2}{\pi i\tau} = \frac{i}{2\hbar t}w^2$, $\frac{z}{\tau} = -\frac{2aw}{\hbar t}$

$-\frac{1}{\tau} = \frac{8a^2}{\hbar\pi t}$, and substituting:

$$\frac{1}{4a}\Theta_3\left(\frac{\pi w}{4a}, -\frac{\hbar\pi t}{8a^2}\right) = \frac{1}{4a}\left(\frac{8a^2}{\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{2\hbar t}w^2\right] \times$$

$$\theta_3\left(-\frac{2aw}{\hbar t}, \frac{8a^2}{\hbar\pi t}\right)$$

$$= \left(\frac{1}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{2\hbar t}w^2\right]\sum_{n=-\infty}^{\infty}\exp\left[\pi i\left(\frac{8a^2}{\hbar\pi t}\right)n^2\right]\exp\left[2ni\left(-\frac{2aw}{\hbar t}\right)\right]$$

$$= \left(\frac{1}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{2\hbar t}w^2\right]\sum_{n=-\infty}^{\infty}\exp\left[\left(\frac{i}{2\hbar t}\right)(16a^2n^2 - 8anw)\right]$$

$$= \left(\frac{1}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{2\hbar t}w^2\right]\sum_{n=-\infty}^{\infty}\exp\left(\left(\frac{i}{2\hbar t}\right)((4an-w)^2 - w^2)\right)$$, Thus

(2.6) $$\sum_{n=-\infty}^{\infty}\left(\frac{1}{2\pi i\hbar t}\right)^{1/2}\exp\left[\frac{i}{\hbar}\frac{1}{2}\frac{(4an-w)^2}{t}\right] = \frac{1}{4a}\Theta_3\left(\frac{\pi w}{4a}, -\frac{\hbar\pi t}{8a^2}\right)$$

Using (2.2), we write $\frac{1}{4a}\Theta_4\left(\frac{\pi(x+y)}{4a}, -\frac{\hbar\pi t}{8a^2}\right)$

$$= \frac{1}{4a}\Theta_3\left(\frac{\pi(x+y)}{4a} + \frac{\pi}{2}, -\frac{\hbar\pi t}{8a^2}\right) = \frac{1}{4a}\Theta_3\left(\frac{\pi(x+y+2a)}{4a}, -\frac{\hbar\pi t}{8a^2}\right)$$

Finally, applying (2.6) to to (2.5) with $w = x-y$, $w = x+y+2a$ we arrive at:

$$\underline{(2.7)}\quad K_t(x,y) = \sum_{n=-\infty}^{\infty} \left(\frac{1}{2\pi i\hbar t}\right)^{1/2} \exp\left(\frac{i}{\hbar}\frac{1}{2}((x-4an)-y)^2\right) - \sum_{n=-\infty}^{\infty}\left(\frac{1}{2\pi i\hbar t}\right)^{1/2} \exp\left(\frac{i}{\hbar}\frac{1}{2}((4n-2)a-x-y)^2\right)$$

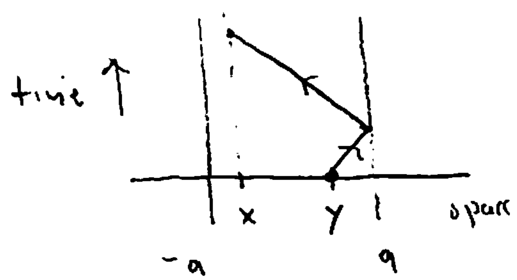
Now, on $\mathbb{R}$ the expression for the free particle kernel is

$$K_t^F(x,y) = \left(\frac{1}{2\pi i\hbar t}\right)^{1/2} \exp\left[\frac{i}{\hbar}\frac{1}{2}\frac{(x-y)^2}{t}\right]$$ $\therefore$ (2.7) can be written:

$$\boxed{\underline{(2.8)}\; K_t(x,y) = \sum_{n=-\infty}^{\infty} K_t^F(x+4na, y) - \sum_{n=-\infty}^{\infty} K_t^F(-x+2a+4na, y)}$$

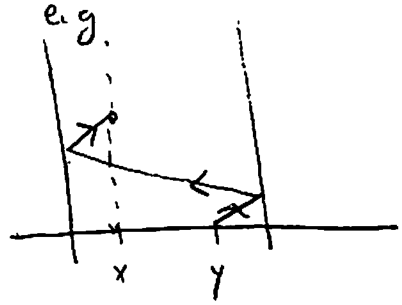
3. Interpretation of the result

It is helpful to represent motion in the classical system B with space-time diagrams: e.g.



one collision

or



two collisions, etc.

Let R = reflection wrt $x=a$ line: $R(x) = -x+2a$
S = reflection wrt $x=-a$ line: $S(x) = -x-2a$

and let $T = R\circ S = x+4a$. Let G = gp generated by R and S

It is easy to check the following relations:

$$R^2 = S^2 = e \ , \quad T \cdot R = RT^{-1} , \quad TS = R$$

which imply that every element of G has a unique expression of the form T^n, or RT^n, $n \in \mathbb{Z}$. Furthermore, G acts on $\mathbb{R}^1$ and I represents a fundamental domain for this action:

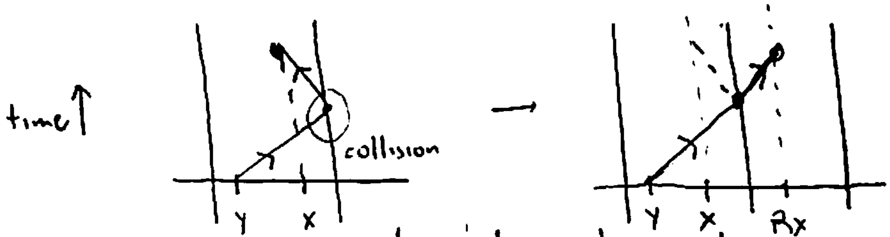
$$\cdots \underset{-3a}{+} \ RT^{-1} \ \underset{-a}{+} \ e \ \underset{a}{+} \ R \ \underset{3a}{+} \ T \ \underset{5a}{+} \ RT \ \underset{7a}{+} \ T^2 \ + \cdots \quad \text{etc.}$$

where we've labelled the intervals with the group element that maps I to it.

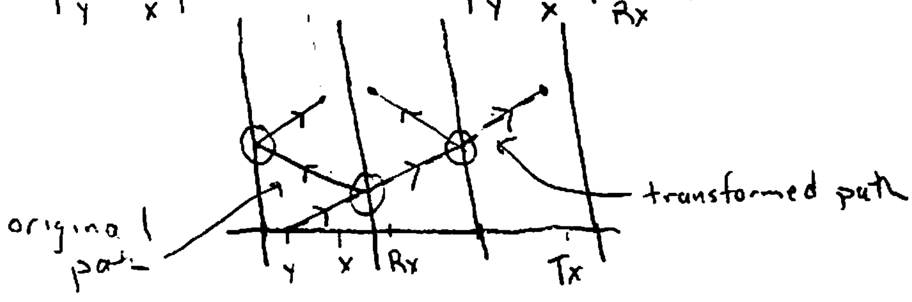
Next, let $\chi : G \to \mathbb{C}^\times$ be a complex homomorphism. χ is determined by its values $\chi(S)$, $\chi(R)$ ($= \pm 1$ since $S^2 = R^2 = e$). Fix χ by $\chi(S) = \chi(R) = -1$. Then $\chi(T^n) = 1$, $\chi(RT^n) = -1$ and we can compactly write the result (2.8):

$$(\underline{3.1}) \qquad K_t(x,y) = \sum_{g \in G} \chi(g) \, K_t^F(g \cdot x, y).$$

Next we consider a mapping of the path space of B, $\mathcal{P}(B)$, to the path space of $\mathbb{R}$, $\mathcal{P}(\mathbb{R})$: for every collision of a path on B with the boundary, we reflect the rest of path wrt that boundary. Polygonal paths are mapped to polygonal paths, and free particle motions are preserved. Eg:



and



Notice this maps paths in B with (start, end) = (y, x) into paths in $\mathbb{R}$ with (start, end) = $(y, x+4na)$ or $(y, -x+2a+4na)$ $n \in \mathbb{Z}$. For an even # of collisions, end = $x+4na$; for an odd #, end = $-x+2a+4na$.

Consider a polygonal path γ in $\mathbb{R}$ with endpoints (y, w). For each intersection with the lines $x = \pm(2n+1)a$, $n = 0, 1, 2, \ldots$ we assign an intersection # $+1$, if the intersection is in the positive sense, -1 otherwise, where

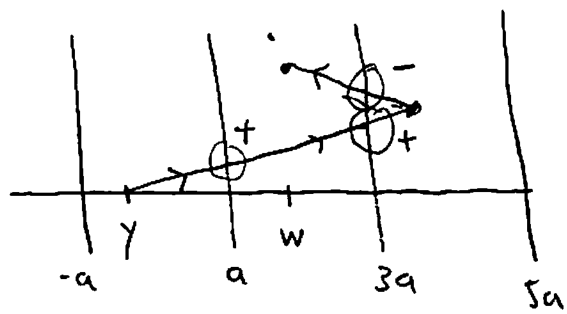
↑ time

 = + sense ,  = − sense.

space →

(We are assuming γ is transverse to these lines – the parts of γ not transverse do not contribute any action. A more sophisticated analysis would be concerned with this point)

Eg.



No matter how the curve meanders around, the sum (or product) of the algebraic intersection numbers is a function solely of the endpoints. If $I(w, y)$ = Σ algebraic intersection numbers, then we have the formula $(-1)^{I(gx, y)} = \chi(g)$, $g \in G$. Alternately, let $\gamma' \in \mathcal{P}(B)$ and $\gamma \in \mathcal{P}(\mathbb{R})$ denote its image under this mapping. If γ has endpoint $g \cdot x$, then

$$\chi(g) = \begin{cases} +1 & \text{if } \gamma' \text{ has an even \# of collisions} \\ -1 & \text{if } \gamma' \text{ has an odd \#} \end{cases}$$

Putting this all together, we can suggest interpreting the right hand side of (3.1) as representing a Feynman sum over the transformed paths in $\mathbb{R}$, with a phase factor of $\chi(g)$ inserted for paths ending at $g \cdot x$. Using Feynman's notation [2],

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we would write (3.1) as:

$$\text{(3.2)}\quad K_t(x,y) \equiv \int_{\substack{\gamma'(0)=y \\ \gamma'\in \mathcal{P}(B)}}^{\gamma'(t)=x} e^{\frac{i}{\hbar}S(\gamma')}\,\mathcal{D}(\gamma') = \sum_{g\in G} \int_{\substack{\gamma(0)=y \\ \gamma\in \mathcal{P}(\mathbb{R})}}^{\gamma(t)=g\cdot x} \chi(g)\, e^{\frac{i}{\hbar}S(\gamma)}\,\mathcal{D}(\gamma)$$

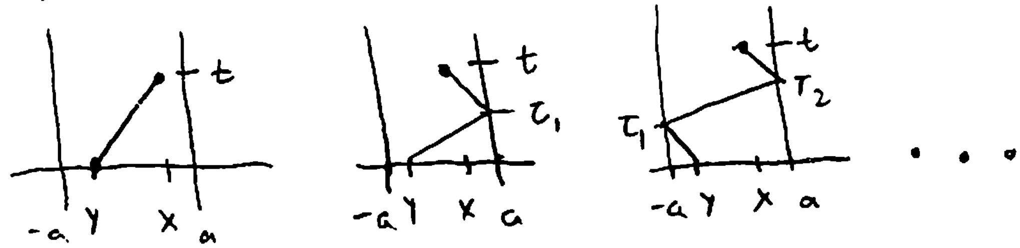
However, the classical action, $S(\gamma')$, for γ' is the same as the classical action, $S(\gamma)$, for the transformed path. Why then the factor $\chi(g)$?

4. The factor $\chi(g)$

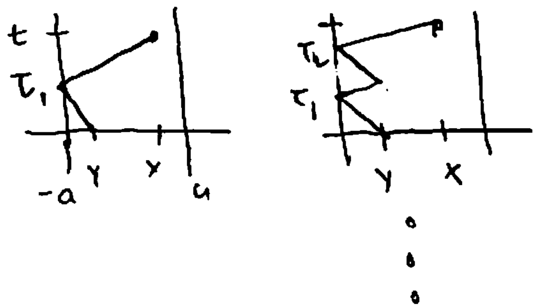
The transformation between paths in B and $\mathbb{R}$, although geometrically simple, is, in fact, quite complicated. We can naively interpret $\chi(g)$ as representing the Jacobian of the transformation $\gamma' \to \gamma$, i.e. $\mathcal{D}(\gamma') \mapsto \chi(g)\,\mathcal{D}(\gamma)$. To make this precise, one would have to expand the sum in (3.2) in terms of a perturbation series:

$$\int_{\gamma'\in\mathcal{P}(B)} = \int_{\substack{\gamma'\in\mathcal{P}(B) \\ 0 \text{ collisions}}} + \int_{\substack{\gamma'\in\mathcal{P}(B) \\ 1 \text{ collision}}} + \int_{\substack{\gamma'\in\mathcal{P}(B) \\ 2 \text{ collisions}}} + \cdots$$

, represented as



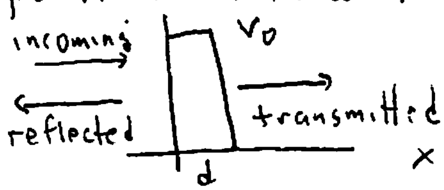
Note that each diagram transforms to free particle diagrams on $\mathbb{R}$ using a time ordered sequence of transformations from G.



(9) Particle in a box (cont.) Aaron Hershman

Although this is the start of a rigorous approach, we will not persue it further, since it is better dealt with by more sophisticated techniques. Instead we will content ourselves with assuming that only the total # of collisions enters into the factor and not their order or which boundary they occur at.

Consider a collision experiment with a finite height potential barrier



In a scattering experiment, we assume the particle is asymptotically free for large values of $|x|$. Following Schiff [ ], we represent a wave function $u(x)$ of definite energy $E < V_0$ by

$$u(x) = A e^{ikx} + B e^{-ikx} \qquad x \le 0$$
$$= C e^{ikx} \qquad x \geq a$$

Analysis of the prob current density shows it is reasonable to interpret A as the coefficient of the incoming wave, and B as the coefficient of the reflected wave. Thus we can interpret the limit, $\lim_{V_0 \to \infty} \frac{B}{A}$, as the change in phase due to <u>one</u> collision.

Let $\beta = \left[\frac{2m(V_0 - E)}{\hbar^2}\right]^{1/2}$. Then, from Schiff (p 103), we have the formula

$$\frac{B}{A} = \frac{(k^2+\beta^2)(1-e^{-2\beta a})}{(k+i\beta)^2 - (k-i\beta)^2 e^{-2\beta a}}$$

Now $V_0 \to \infty \Rightarrow \beta \to 0 \quad \therefore \quad e^{-2\beta a} \to 0$; dividing both sides by β^2 we conclude $\lim_{V_0 \to \infty} \frac{B}{A} = -1$

This justifies the formula for $\chi(g)$ and concludes the derivation.

5. References

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Received: from math.berkeley.edu by violet.berkeley.edu (8.6.8/1.33r)id WAA23114; Mon, 16 May 19
lupEudora by violet.berkeley.edu (8.6.8/1.33r)id WAA23101; Mon, 16 May 1994 22:17:10 -0700 Message-Id: <199405170517.WAA23101@violet.berkeley.edu> X-mailer: Eudora 1.3
Date: Mon, 16 May 1994 22:20:38 -0800
To: marsden@math.berkeley.edu
From: aaronjh@violet.berkeley.edu (Aaron Hershman) Subject: LonM typos

Dear Jerry,

I've sent you a fax with some corrections to Chp 3 that were not on the other list. Let me know if you don't receive the fax.

I got the paper by Renete Loll (actually 2 papers) that you were looking for. If you can't find your copy, I can lend you this one. It looks very interesting.

I have a lot of things to talk about with you. In the process of working out the particle in a box path integral, I've begun to appreciate the role that complexification seems to be secretly playing. For example, the key steps in that calculation involve various theta function identities - the theta functions are themselves solutions to a Schrodinger equation wrt complex space and time coordinates! So I'm seeing that your initial intuition in that direction was on the mark.

I would like to talk to you about the particle in a box example. By starting with the propagator as derived from the wave equation, I've worked the answer backwards and expressed it as a path integral. This "solves" the problem; the only thing is is that I don't understand how to interpret the path integral! It seems to be a reduction with respect to a non-Abelian discrete group.

(Specifically, let I=[-a,a], R(x)= -2a-x, S(x)= 2a-x. R = reflection wrt -a, S = reflection wrt a; G = affine group generated by S,R; I is a fundamental domain in R^1 for G. I express the path integral on I in terms of path integrals on R^1 and the group action of G).

Anyway, I would like show you how this works and get your input. I won't be back until the 2nd week of June. I'm sorry I'll be missing the beginning lectures for the seminar. Hopefully, someone will be taking good notes.

Sincerely yours,
Aaron